

The concentration parameter thermal microstresses as the thermophysical characteristics of two-phase materials

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Abstract. Thermal strength is one of the main thermophysical characteristics of structural materials. For homogeneous systems it is determined by the strength characteristics of the material. While for inhomogeneous systems, in particular, multiphase ones, it is necessary to consider the nature of the microstructure. Heat resistant real materials such as steels are known to be multi-phase systems. One of the mechanisms of their destruction is associated with the presence of propagating heat fluxes that generate thermal stresses. The aim of this paper is to evaluate the patterns of the formation of spatial distributions of thermal stresses in matrix systems of round inclusions characterized by different mutual disposition. The spatial distributions of thermal stresses in a two-phase material characterized by a matrix structure with round inclusions are investigated. For the numerical solution of the problem of stationary thermal conductivity the finite element method with discretization of the medium by triangular elements is used. It was found that at certain points in the medium the values of thermal stresses are ten times higher than the average for the material. It is shown that the spatial distribution and the local magnitude of the temperature gradient depend on the shape of the particles of the phase components and the values of their thermal conductivities. It is considered that the elastic moduli of inclusion and matrix differ little from each other.

1. Introduction

The paper draws attention to the need to take into account the inhomogeneous character of the distribution of thermal stresses in two-phase materials. The spatial distributions of thermal stresses in a two-phase material characterized by a matrix structure with round inclusions are investigated.

For numerical modeling the finite element method with discretization of the medium by triangular elements was used. It was found that at certain points in the medium the values of thermal stresses are tens of times higher than the average values for the material [6].

One of the main thermophysical characteristics of constructional materials is the thermal resistance. For homogeneous systems it is determined by the strength characteristics of the material. However, for heterogeneous systems, in particular multiphase ones, it is necessary to take into account the nature of



the microstructure. Heat resistant real materials such as steels are known to be multi-phase systems. One of the mechanisms of their destruction is associated with the presence of propagating heat fluxes that form thermal stresses. The paper shows that the spatial distribution and the local value of the temperature gradient depend on the shape of particles of the phase components and values of their thermal conductivities. The schemes of microstructures of the systems under consideration are shown in Fig. 1.

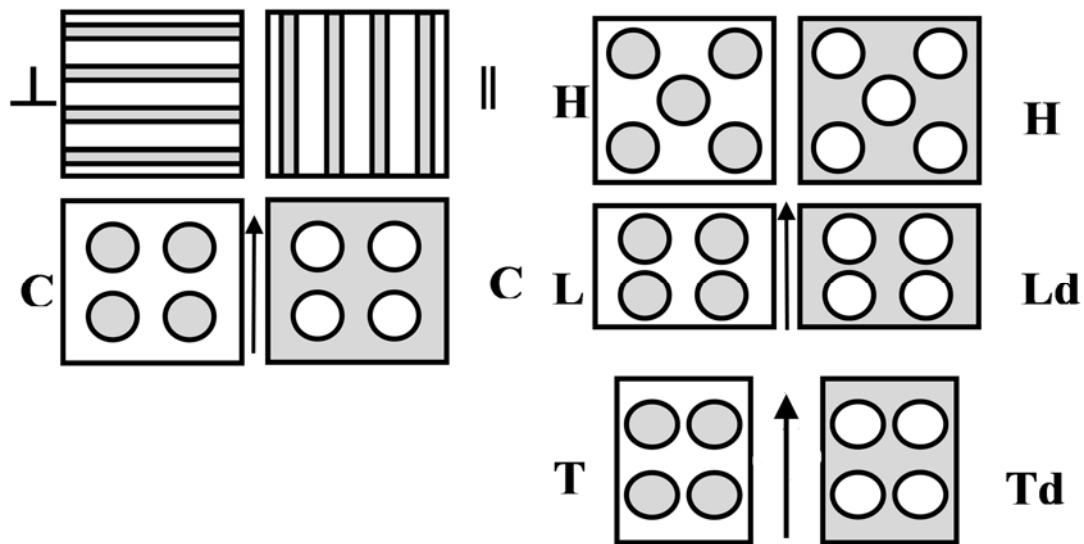


Figure 1. The schemes of structures (dark colour).

The investigated effect of the concentration is expediently to be illustrated by the example of layered systems consisting of regions with a different value of thermal conductivity (in Fig. 1, the systems are designated « \perp » and « \parallel » respectively).

Figure 1 shows when the heat is propagated perpendicular to the layers, the conductive system can be approximated by a series connection of thermal resistances. In this case, the values of the temperature gradients g_k in the layers will be inversely proportional to their thermal conductivity coefficients σ_k of the layer materials, i.e. there is a concentration of thermal stresses in the layers with minimal thermal conductivity. For a given two-phase system, we have

$$\gamma_{\perp} = g_{\max} / g_{\min} = \sigma_{\min} / \sigma_{\max},$$

where the parameter γ characterizes the contrast of the gradients. In the case of the parallel direction of the propagation of the heat flux to the layers' planes, the thermal resistances are switched in parallel, so we have

$$\gamma_{\parallel} = 1$$

that is, the voltages in both phase components are the same. It can be assumed that the values of γ_{\perp} and γ_{\parallel} characterize the "plug" for arbitrary regular matrix two-phase structures. For layered two-phase systems the spectrum of values of the temperature gradients realized in the sample has the form of delta-like functions. It was shown earlier [3, 4, 7] that in the case of matrix two-phase regular structures, such spectra are characterized by a complex shape and determined by the spatial inhomogeneity of the heat fluxes.

The purpose of this paper is to evaluate the patterns of the formation of spatial distributions of thermal stresses in matrix systems of round inclusions characterized by different mutual disposition (Fig. 1). The structures on the left and on the right are dual to each other, that is, they are obtained by

rearranging the phase and inclusions materials and rotating by 90°. The arrow shows the flow direction. We consider stationary processes of heat conduction and assume that the elastic moduli of inclusion and matrix are not much different from each other. Under these conditions, the local values of the thermal stresses are proportional to the magnitude of the temperature gradient at a given point.

2. Method of thermal stresses calculation

To calculate the temperature distribution in the spatially inhomogeneous systems under consideration, we use the finite elements method [1-4, 7]. We note the general features of the method.

A plane-symmetric heat transfer process is considered. To find the spatial distribution of temperature φ , we use an approach based on the variation formulation of the transfer equations and the finite elements method. In addition we use the condition of extremality of the functional:

$$\chi = \int_{S_c} \sigma(\text{grad } \varphi)^2 dS$$

where S_c is the area of the unit cell. The conditions for the minimum of the functional χ make it possible to establish the nodal values of the temperature at all points of the unit cell and, correspondingly, the magnitude of the temperature gradients. To solve this problem, a computer program was developed in the FORTRAN language and a series of computer experiments was carried out [7].

In the calculations we consider a two-dimensional plane process of heat propagation in a rectangular unit cell containing some quarters of the inclusions. On the boundaries of the rectangular calculated domain, we take isothermal and adiabatic boundary conditions. For the discretization of the area we use grid of partitions with a density of 100x100 elements.

3. Results of calculations of thermal stresses

Analysis of the calculation results shows a significant heterogeneity in the distribution of the parameter γ (x, y). At different points of the material, regions with a reduced ($\gamma < 1$) and elevated values ($\gamma > 1$) of thermal stresses in comparison with the homogeneous case are realized. In this case, the pattern of distribution of thermal stresses essentially depends on the type of structure and differs for mutual-dual structures. Various points of localization of stresses of their magnitude are observed.

Let us consider systems of round inclusions that differ from each other by the ratio of the conductivity of the matrix and the inclusion, the concentration (radius) of inclusion and the location of the inclusions with respect to each other. We assume that the conductivities of the matrix and the inclusions differ by 100, 10 and 2 times. This corresponds to the characteristic values inherent in various classes of real materials, for example, the phase component of steels. We will take into account that the particles can be located evenly, forming a square lattice, either in staggered order, or assembled in groups, forming thickening or perpendicular, or parallel to the direction of flow propagation.

Consider a system C in which the particles are conducting, and the matrix is an insulating one. The conductivities of the matrix and the inclusion are $\sigma_{\text{matr}} = 0.01$; $\sigma_{\text{BKL}} = 1$, respectively, and the inclusion radius $R_{\text{BKL}} = 0.7$, which corresponds to the concentration $C_{\text{vkl}} = 38\%$. The schemes of calculation areas are shown in the sidebar to Figures 2 and 3. Let us trace the changes in the thermodynamic potential (temperature) along the dashed lines in the cell diagram. They correspond to straight lines $y = 0.5$ and $x = 0$, respectively.

The main field (Figure 2) shows the characteristic dependences of the potential φ , established for the values $y = 0.5$ and $x = 0$ ($\varphi(x)$ and $\varphi(y)$, respectively).

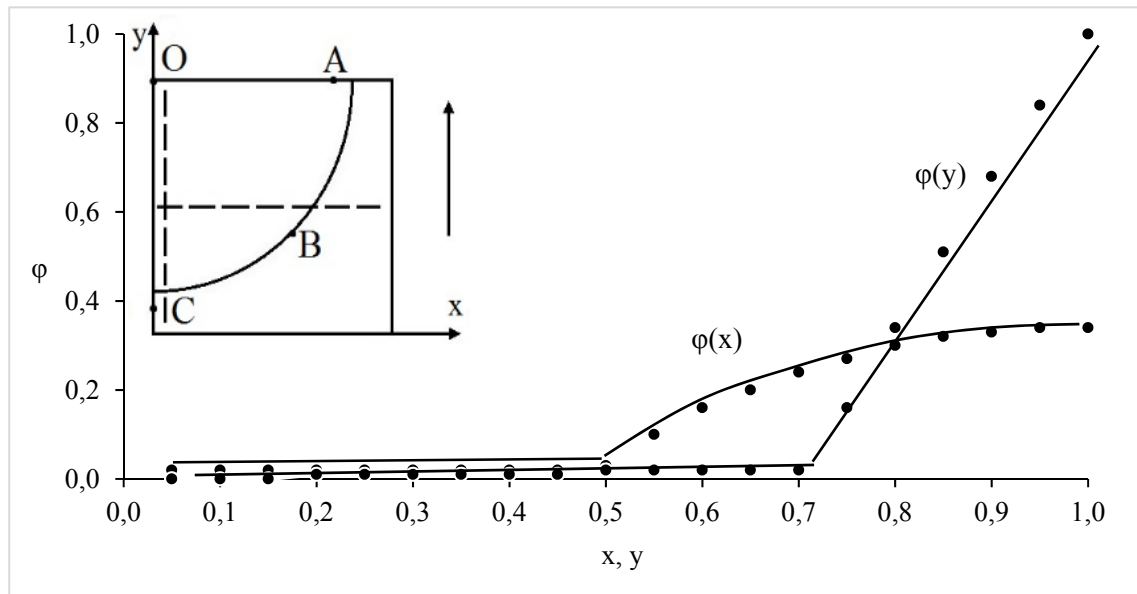


Figure 2. The distribution of the thermodynamic potential $\varphi(x)$ and $\varphi(y)$; Dashed lines on the sidebar - directions of scans; O, A, B, and C are the characteristic points of the medium

Inside the inclusion (x, y in the neighborhood of zero) the potential is close to zero and is constant, that is, the gradient of the potential $g = \text{grad}(\varphi)$ is close to zero. Upon exiting the inclusion, fractures are revealed, which indicate a sufficiently noticeable change in the gradient of the potential during the transition from the inclusion to the matrix (Figure 2).

Figure 3 shows the characteristic dependences of the gradient $g(x)$ and $g(y)$, corresponding to Figure 2.

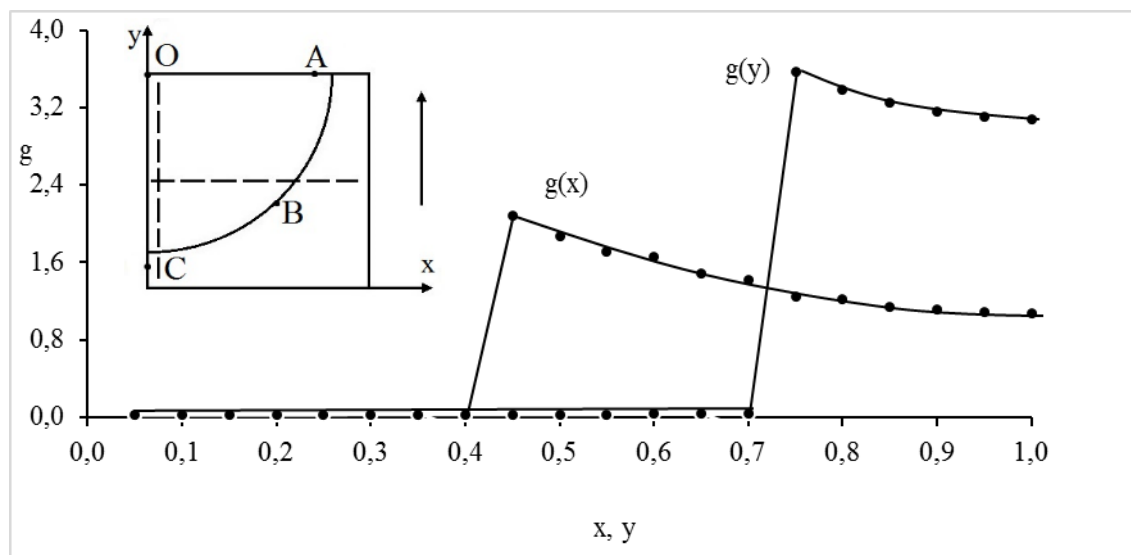


Figure 3. The distribution of the relative gradient of the potential $g(x)$ and $g(y)$; Dashed lines on the sidebar to the drawing - directions of scans; O, A, B, and C are the characteristic points of the medium.

To analyze the behavior of the temperature gradients with variations in the concentration of inclusions and the thermal conductivities of the matrix and the inclusion we choose the most significant points "C" and "O" in the structure of "C" (Figure 4). The area of the matrix, located "below" the inclusion corresponds to point "C" and the center of the particle corresponds to the point "O".

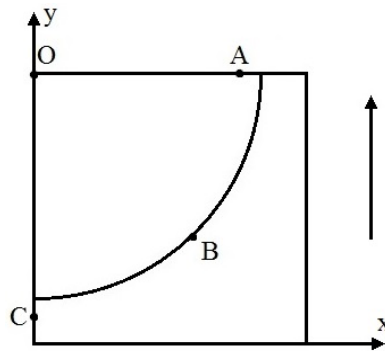


Figure 4. The scheme of the unit cell. The arrow is the direction of heat flow distribution

The analysis of the obtained data showed that in the situations under consideration a substantial heterogeneity of the spatial distribution of the potential is observed. In this case, the concentration of the potential gradient was found at point "C", in which it has the maximum value. It exceeds the value that is inherent in a homogeneous sample more than 70 times.

Figure 5 shows the graphs of the dependence of these values on the concentration of inclusions with a conductivity ratio of 100 times.

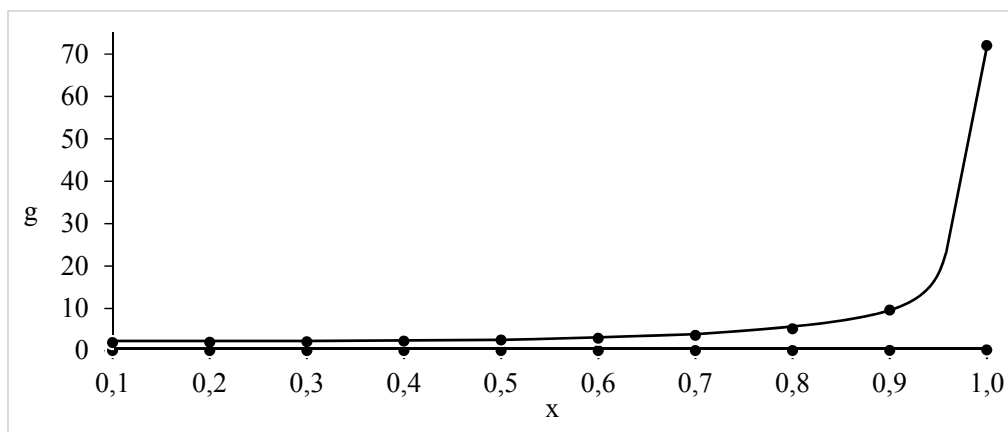


Figure 5. Structure C, matrix conductivity $\sigma_{\text{matr}} = 0.01$, conductivity of inclusion $\sigma_{\text{BKЛ}} = 1$. Conductivity ratio $\sigma_{\text{BKЛ}} / \sigma_{\text{matr}} = 100$. The upper curve corresponds to the values of the gradient g at the point "C", the lower curve corresponds to the point "O"

At the center of the conducting inclusion the gradient has a very small value of 0.02. Consequently, at the point "O" the thermal stresses are negligibly small. The heat flux propagates through the inclusion and the gradient is concentrated at the point "C", because the conductivity of the matrix is less than the conductivity of the inclusion 100 times.

At the point "C" in the diluted system (the radius of inclusion R is of the order of 0.1- 0.3) the gradient is practically constant and has a value of the order of 2.0. As the inclusion concentration rises within $R = 0.3- 0.8$, the gradient gradually grows to about 5, and then a sharp increase to values of the order of 72 is observed. Figure 6 shows the dependence of the gradient g on the concentration of inclusions at a conductivity ratio of 10 times.

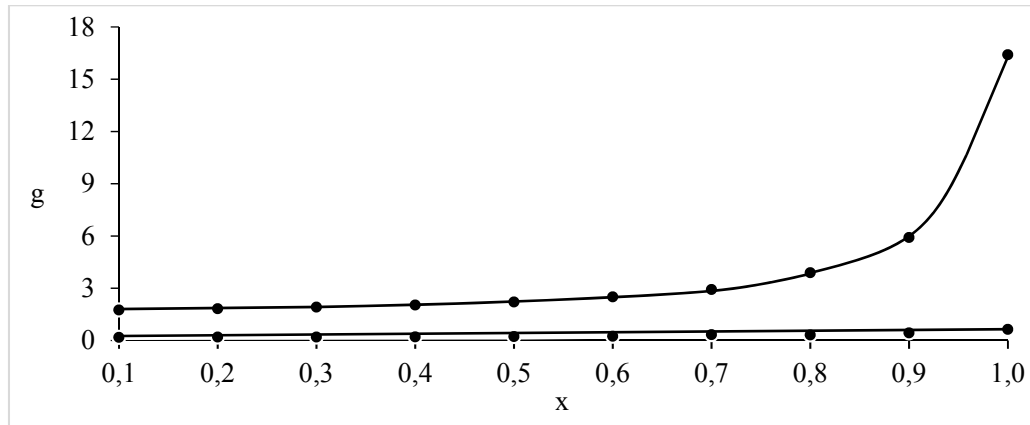


Figure 6. Structure C, matrix conductivity $\sigma_{\text{matr}} = 0.1$, conductivity of inclusion $\sigma_{\text{BKЛ}} = 1$. Conductivity ratio $\sigma_{\text{BKЛ}} / \sigma_{\text{matr}} = 10$. The upper curve corresponds to the values of the gradient g at the point "C", the lower curve corresponds to the point "O"

At the center of the conducting inclusion the gradient has a very small value of 0.2. Hence, there are no thermal stresses. At the point "C" in the diluted system (R of the order of 0.1- 0.3) the gradient has a value of about 1.8. As the inclusion concentration rises within $R = 0.3- 0.8$, the gradient gradually increases from 2 to 3.9. A sharp increase is observed at a radius of $R \rightarrow 1$ to a value of 16.4.

With a decrease in the conductivity ratio from 100 to 10, the values of the gradient g decrease proportionally at the point "C" and increase at the center of the inclusion (at the point "O").

Figure 7 shows the dependence of the gradient g on the inclusion concentration at a conductivity ratio of 2 times.

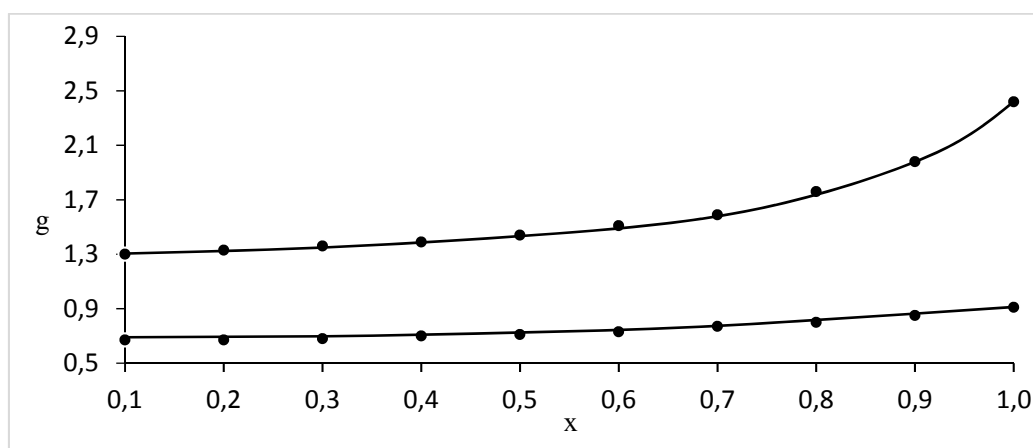


Figure 7. Structure C, matrix conductivity $\sigma_{\text{matr}} = 0.5$, conductivity of inclusion $\sigma_{\text{BKЛ}} = 1$. Conductivity ratio $\sigma_{\text{BKЛ}} / \sigma_{\text{matr}} = 2$. The upper curve corresponds to the values of the gradient g at the point "C", the lower curve corresponds to the point "O"

At the center of the conducting inclusion at the point "O", the gradient has a small value of about 0.7. At the point "C" in the diluted system (R of order 0.1- 0.3), the gradient is 1.3. As the concentration of inclusion increases, a gradual increase to a value of the order of 2 occurs.

With a decrease in the conductivity ratio from 10 to 2, the gradient values decrease proportionately at the point "C" and increase at the center of the inclusion (at the point "O"). Therefore, in the structure C, the most dangerous situation is with an inclusion concentration, where $R \rightarrow 1$, and with a conductivity ratio $\sigma_c / \sigma_{\text{matr}} = 100$. In this case, a crack at the point "C" is the most likely to occur.

When the inclusion has an increased conductivity and the matrix has a reduced conductivity, there is a general tendency to concentrate the gradient in the matrix region.

In the process of closing inclusions, the gradient grows significantly and concentrates at the point "C". This is because the heat flux propagating through the inclusion meets the barrier in the form of a weakly conducting matrix at the point "C". Therefore, the maximum gradient g is observed at the inclusion radius $R \rightarrow 1$.

Consider the dual structures Cd. They differ from the original ones by mutual replacement of the material of matrix and inclusion. In the structure of Cd, the matrix is conductive, and the inclusion is an isolating. To analyze the regularities in the structure of Cd, we select the most significant points "A" and "O". Point "A" corresponds to the region of the right boundary of the inclusion.

The results of the investigation when a conductivity ratio is 100 are shown in Figure 8.

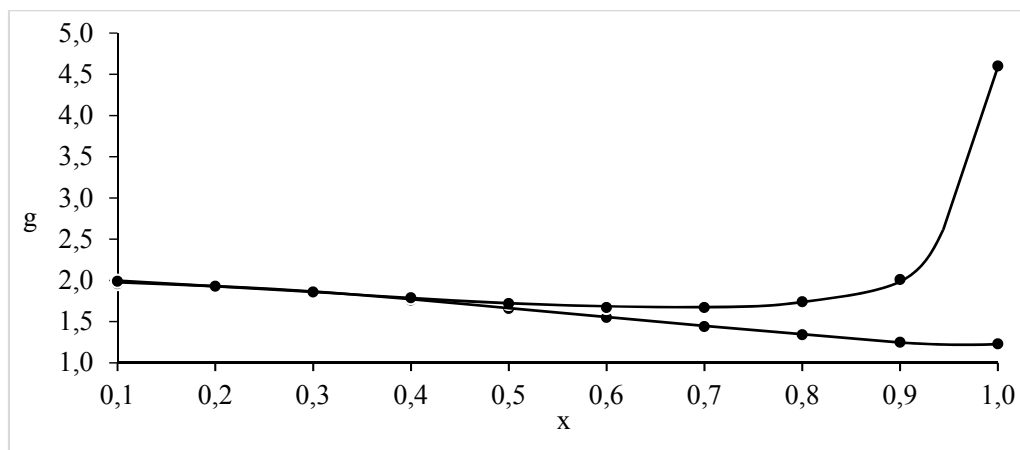


Figure 8. Dual structure Cd, matrix conductivity $\sigma_{\text{matr}} = 1$, conductivity of inclusion $\sigma_{\text{вкл}} = 0.01$. Conductivity ratio $\sigma_{\text{вкл}} / \sigma_{\text{matr}} = 100$. The upper curve corresponds to the values of the gradient g at the point "A", the lower curve corresponds to the point "O"

The heat flux propagates through the matrix, bypassing the inclusion, since the conductivity of the inclusion is less than the conductivity of the matrix 100 times. As the concentration of inclusion increases, the gradient gradually decreases in the center of the weakly conducting inclusion (at the point "O").

In a diluted system ($R = 0.1 - 0.3$) the gradient value is almost constant at both the "O" point and the "A" point and has a value of 1.8. As the particle concentration increases from 0.4 to 0.6, the gradient decreases to 1.67. At a particle concentration $R = 0.6 - 0.7$, a minimum of the gradient g is observed due to the transition from a homogeneous field in the inclusion to the inhomogeneous field. As the concentration rises within $R = 0.7 - 1$, the gradient grows to a value of the order of 5. The maximum value of the gradient g is observed at the point "A" when $R \rightarrow 1$, because the distance between the particles decreases and the propagation of the heat flux becomes more difficult.

We now turn to the calculation results, where the conductivity ratio is 10.

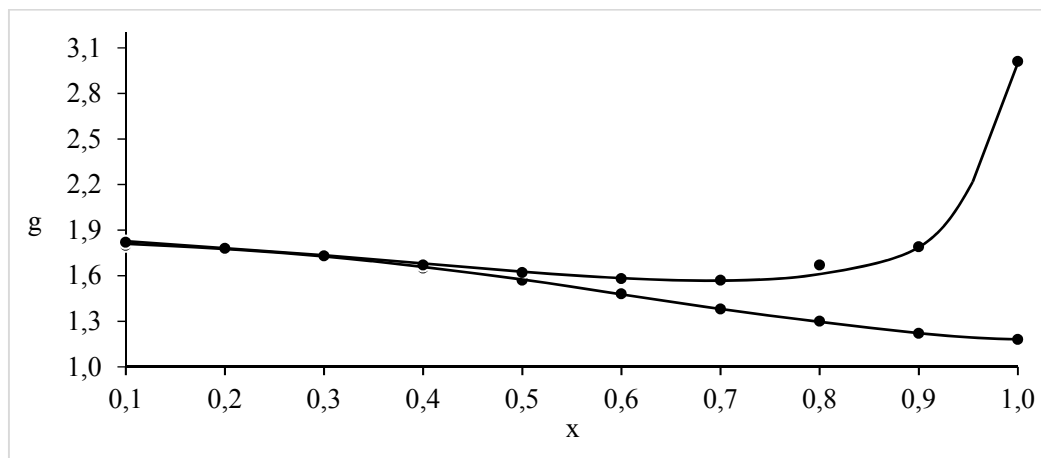


Figure 9. Dual structure Cd, matrix conductivity $\sigma_{\text{matr}} = 1$, conductivity of inclusion $\sigma_{\text{вкл}} = 0.1$. Conductivity ratio $\sigma_{\text{вкл}} / \sigma_{\text{matr}} = 10$.

In the center of the inclusion at the point "O", as the concentration of inclusion increases, the gradient gradually decreases. This is because the heat flow spreads through the matrix, bypassing the inclusion.

In a diluted system ($R = 0.1 - 0.3$) the gradient value is almost constant at both the "O" point and the "A" point and has a value of about 1.7. When the inclusion concentration is $R = 0.4 - 0.7$ the gradient g decreases to 1.57, where a minimum in connection with the transition from a homogeneous field to an inhomogeneous field is observed. As the inclusion concentration rises within $R = 0.7 - 1$, a gradual growth of the gradient to a value on the order of 3 occurs.

When the conductivity ratio decreases from 100 to 10, the values of the gradient g decreases proportionally both at the point "A" and at the center of the inclusion (at the point "O").

Figure 10 shows the dependence of the gradient g on the inclusion concentration at a conductivity ratio of 2.

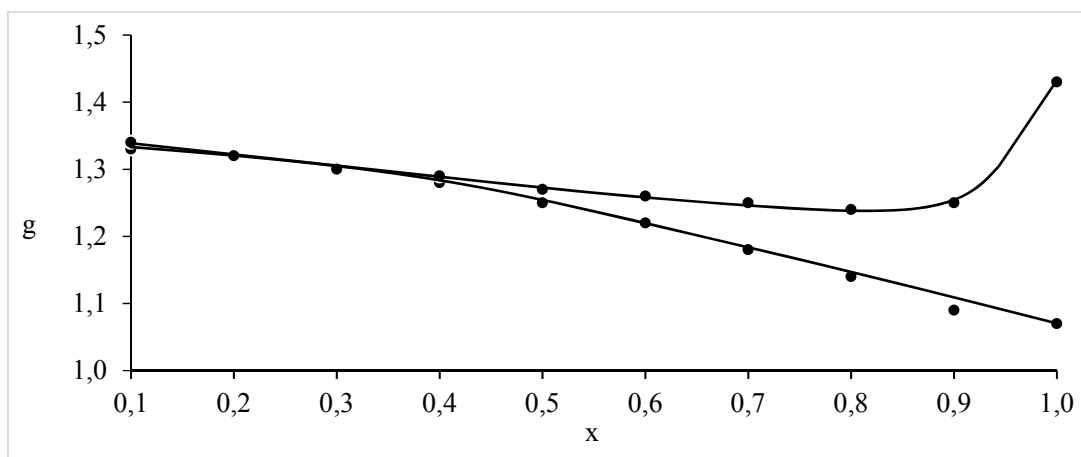


Figure 10. Dual structure Cd, matrix conductivity $\sigma_{\text{matr}} = 1$, conductivity of inclusion $\sigma_{\text{вкл}} = 0.5$. Conductivity ratio $\sigma_{\text{вкл}} / \sigma_{\text{matr}} = 2$.

At the center of the inclusion, as the concentration increases, the gradient gradually decreases due to the fact that the heat flux propagates through the matrix. In a diluted system ($R = 0.1 - 0.3$), the gradient value is almost constant at both the "O" and "A" points and has a value of 1.3.

As the inclusion concentration increases from $R = 0.3$ to 0.8 , the gradient value at point "A" is almost constant and has a value of 1.25 . The minimum is observed at a concentration of $R = 0.8$ and is 1.24 .

With the inclusion concentration $R \rightarrow 1$, the gradient increases to 1.45 at the point "A". When the conductivity ratio decreases from 10 to 2 , the values of the gradient of φ decrease proportionally both at the point "A" and point "O", which is the center of the inclusion. Consequently, a dangerous situation arises at the highest inclusion concentration where the radius is $R \rightarrow 1$ and with a maximum conductivity ratio of 100 . The crack is most likely to occur at the point "A" on the left and right boundaries of inclusion.

In the case of the dual structure Cd, when the inclusion has a lower conductivity, there is a general tendency to concentrate the gradient in the left and right inclusion regions. At low concentrations the field is known to tend to homogeneity inside the inclusion (the constancy of the gradient g).

In the process of the inclusions closing the field pattern changes. The gradients are concentrated at the point "A". This is because the streamlines flowing around the inclusion concentrate in it.

Analyzing the value of the gradient g , realized at the points "O" and "A" in dependence on the inclusion concentration, one can observe a minimum. It is explained by the transition from a homogeneous field in the inclusion to the inhomogeneous field.

Figure 11 shows typical patterns of spatial distributions $g(x, y)$ of systems C and Cd. The lines near inclusions limit the regions that differ by g values by a factor of two.

Analysis of the calculation results shows that for the system C ("conducting inclusions") the heat flow lines are contracted into conducting particles, while the thermal stresses are concentrated in the interval between the particles and directed "parallel" to the general direction of flow propagation (Figure 2). For the dual system Cd streamlines are preferably in a conductive matrix around the inclusion and the thermal stress maximum is in the transverse direction. In the case of conducting inclusions "C", maximum gradient γ_{\max} reach several tens of magnitude (at $\sigma_2 / \sigma_1 = 100$). At the same time these values for the Cd system are several units.

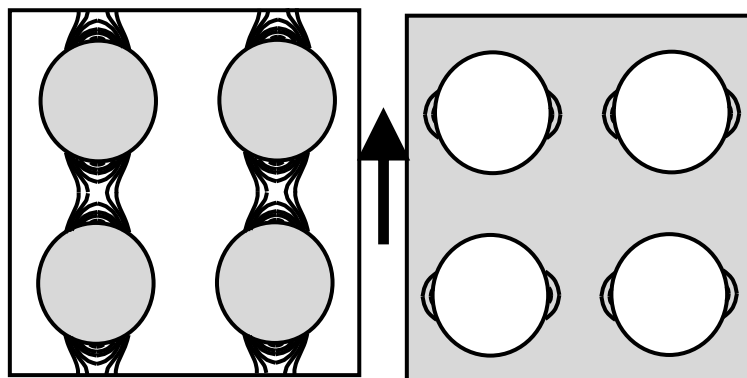


Figure 11. Configurations of the thermal stresses concentration regions in system C, dark color corresponds high-conductivity phase

Using this method we can consider the behavior of the gradient in other structures shown in Figure 1. Analysis of these structures made it possible to reveal some basic regularities of the distribution of the gradient of the thermodynamic potential (temperature) as a concentrator of thermal microstresses.

4. The main regularities of the thermal stress concentrators formation

Investigation of the regularities of the thermal stresses formation in inhomogeneous materials requires further work. Systematizing the data obtained so far, we can arrive at the following conclusions.

1) In the discussed situations, the values of the maximum local thermal stresses depend on the ratio of the phase conductivities, their concentrations and the geometric factors of the microstructure. The values of stress concentration can reach tens of values. One can introduce a parameter characterizing

the influence of the microstructure and the contrast of the thermal conductivities of the components, equal to the ratio of the maximum local and nominal temperature gradients $\gamma = g_{\max}/g_0$. The parameter discussed can be established by calculation and phenomenologically

2) When stationary thermal stresses arise, the most dangerous situation is when the weakly conducting phase forms a matrix, and the high-conductivity component is concentrated in the inclusions.

3) The influence of the geometry of the conducting medium can be presented in the following hierarchy of γ quantities:

$$L > C > H > Td > Cd > Hd > T > Ld$$

4) When analyzing the thermal strength, it is necessary to take into account the peculiarities of inclusion complexes, since they can substantially enhance their influence mutually.

5) Effects of the geometry influence can be significant for predicting the mechanisms of crack formation and scenarios of thermal destruction of two-phase material.

5. References

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